

# Towards Large-Scale Approximation Of Tasks With Derivatives - A Kernel Perspective

Zoltán Szabó – CMAP, École Polytechnique

Joint work with:

- Linda Chamakh [@](#) CMAP & BNP Paribas
- Emmanuel Gobet [@](#) CMAP

M3HPCST,  
Ghaziabad, India  
January 9, 2020

- Def-1 (**feature space**):

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

- Def-1 (feature space):

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

- Def-2 (reproducing kernel):

$$k(\cdot, x) \in \mathcal{H}, \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

Constructively,  $\mathcal{H}_k = \overline{\{\sum_{i=1}^n \alpha_i k(\cdot, x_i)\}}.$

- Def-1 (feature space):

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

- Def-2 (reproducing kernel):

$$k(\cdot, x) \in \mathcal{H}, \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

Constructively,  $\mathcal{H}_k = \overline{\{\sum_{i=1}^n \alpha_i k(\cdot, x_i)\}}.$

- Def-3 (Gram matrix):  $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \in \mathbb{R}^{n \times n} \succeq 0.$

- Def-1 (feature space):

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

- Def-2 (reproducing kernel):

$$k(\cdot, x) \in \mathcal{H}, \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

Constructively,  $\mathcal{H}_k = \overline{\{\sum_{i=1}^n \alpha_i k(\cdot, x_i)\}}.$

- Def-3 (Gram matrix):  $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \in \mathbb{R}^{n \times n} \succeq 0.$
- Def-4 (evaluation):  $\delta_x(f) = f(x)$  is continuous for all  $x$ .

# Kernel, RKHS: generalized inner product, -linear methods

- Def-1 (feature space):

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

- Def-2 (reproducing kernel):

$$k(\cdot, x) \in \mathcal{H}, \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

Constructively,  $\mathcal{H}_k = \overline{\{\sum_{i=1}^n \alpha_i k(\cdot, x_i)\}}.$

- Def-3 (Gram matrix):  $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \in \mathbb{R}^{n \times n} \succeq 0.$
- Def-4 (evaluation):  $\delta_x(f) = f(x)$  is continuous for all  $x$ .

- All these definitions are equivalent,  $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$ .

## Kernel examples: $\gamma > 0$ , $p \in \mathbb{Z}^+$

$$\begin{aligned} k_p(\mathbf{x}, \mathbf{y}) &= (\langle \mathbf{x}, \mathbf{y} \rangle + \gamma)^p, & k_G(\mathbf{x}, \mathbf{y}) &= e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2^2}, \\ k_e(\mathbf{x}, \mathbf{y}) &= e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2}, & k_C(\mathbf{x}, \mathbf{y}) &= \frac{1}{1 + \gamma \|\mathbf{x} - \mathbf{y}\|_2^2}, \\ k_L(\mathbf{x}, \mathbf{y}) &= e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_1}, & \dots \end{aligned}$$

# Kernel examples: $\gamma > 0$ , $p \in \mathbb{Z}^+$

$$k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + \gamma)^p, \quad k_G(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2^2},$$
$$k_e(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2}, \quad k_C(\mathbf{x}, \mathbf{y}) = \frac{1}{1 + \gamma \|\mathbf{x} - \mathbf{y}\|_2^2},$$
$$k_L(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_1}, \quad \dots$$

## Today

- $\mathcal{X} = \mathbb{R}^d$ ,
- continuous, bounded, shift-invariant  $k$ .

## Classical problem

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} L(f(\mathbf{x}_i), y_i) + \lambda \|f\|_{\mathcal{H}_k}^2 \quad (\lambda > 0).$$

Examples:

- $L(a, b) = (a - b)^2$ : kernel ridge regression.
- $L(a, b) = |a - b|_\epsilon$ :  $\epsilon$ -insensitive regression.
- $L(a, b) = \max(1 - ab, 0)$ : classification using hinge loss.

# ERM with derivatives

In fact, often the task:

$$\min_{f \in \mathcal{H}_k} C \left( \left\{ \partial^{\mathbf{p}} f(\mathbf{x}_n) \right\}_{\substack{n \in [N] \\ \mathbf{p} \in D_n}}, \|f\|_{\mathcal{H}_k}^2 \right) \quad \partial^{\mathbf{p}} f(\mathbf{x}_n) := \frac{\partial^{p_1 + \dots + p_d} f(\mathbf{x}_n)}{\partial_{x_1}^{p_1} \cdots \partial_{x_d}^{p_d}}.$$

# ERM with derivatives

In fact, often the task:

$$\min_{f \in \mathcal{H}_k} C \left( \left\{ \partial^{\mathbf{p}} f(\mathbf{x}_n) \right\}_{\substack{n \in [N], \\ \mathbf{p} \in D_n}}, \|f\|_{\mathcal{H}_k}^2 \right) \quad \partial^{\mathbf{p}} f(\mathbf{x}_n) := \frac{\partial^{p_1 + \dots + p_d} f(\mathbf{x}_n)}{\partial x_1^{p_1} \cdots \partial x_d^{p_d}}.$$

Examples : semi-supervised learning with gradient information [Zhou, 2008], nonlinear variable selection [Rosasco et al., 2010, Rosasco et al., 2013], learning of piecewise-smooth functions [Lauer et al., 2012], multi-task gradient learning [Ying et al., 2012], structure optimization in parameter-varying ARX processes [Duijkers et al., 2014], density estimation with infinite-dimensional exponential families [Sriperumbudur et al., 2017], Bayesian inference (adaptive samplers) [Strathmann et al., 2015].

## In more detail

- ① Hermite learning with gradient data:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} \left( [f(\mathbf{x}_n) - y_n]^2 + \|f'(\mathbf{x}_n) - \mathbf{y}'_n\|_2^2 \right) + \lambda \|f\|_{\mathcal{H}_k}^2.$$

## In more detail

- ① Hermite learning with gradient data:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} \left( [f(\mathbf{x}_n) - y_n]^2 + \|\mathbf{f}'(\mathbf{x}_n) - \mathbf{y}'_n\|_2^2 \right) + \lambda \|f\|_{\mathcal{H}_k}^2.$$

- ② Nonlinear variable selection:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} [\mathbf{f}(\mathbf{x}_n) - y_n]^2 + \sum_{j \in [d]} \|\partial_j f\|,$$

$$\|g\| = \sqrt{\frac{1}{N} \sum_{n \in [N]} |g(x_n)|^2}.$$

## In more detail

- ① Hermite learning with gradient data:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} \left( [f(\mathbf{x}_n) - y_n]^2 + \|\mathbf{f}'(\mathbf{x}_n) - \mathbf{y}'_n\|_2^2 \right) + \lambda \|f\|_{\mathcal{H}_k}^2.$$

- ② Nonlinear variable selection:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} [f(\mathbf{x}_n) - y_n]^2 + \sum_{j \in [d]} \|\partial_j f\|,$$

$$\|g\| = \sqrt{\frac{1}{N} \sum_{n \in [N]} |g(x_n)|^2}.$$

- ③ Exponential family:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) \propto e^{\langle \boldsymbol{\theta}, \overbrace{\mathbf{T}(\mathbf{x})}^{\text{sufficient statistics}} \rangle}$$

# In more detail

- ① Hermite learning with gradient data:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} \left( [f(\mathbf{x}_n) - y_n]^2 + \|\mathbf{f}'(\mathbf{x}_n) - \mathbf{y}'_n\|_2^2 \right) + \lambda \|f\|_{\mathcal{H}_k}^2.$$

- ② Nonlinear variable selection:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} [f(\mathbf{x}_n) - y_n]^2 + \sum_{j \in [d]} \|\partial_j f\|,$$
$$\|g\| = \sqrt{\frac{1}{N} \sum_{n \in [N]} |g(x_n)|^2}.$$

- ③ Infinite-dimensional exponential family (score matching):

$$p_{\theta}(\mathbf{x}) \propto e^{\langle \theta, \overbrace{\mathbf{T}(\mathbf{x})}^{\text{sufficient statistics}} \rangle} \Rightarrow p_{\mathbf{f}}(\mathbf{x}) \propto e^{\langle \mathbf{f}, k(\cdot, \mathbf{x}) \rangle_{\mathcal{H}_k}}$$

# In more detail

- ① Hermite learning with gradient data:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} \left( [f(\mathbf{x}_n) - y_n]^2 + \|\mathbf{f}'(\mathbf{x}_n) - \mathbf{y}'_n\|_2^2 \right) + \lambda \|f\|_{\mathcal{H}_k}^2.$$

- ② Nonlinear variable selection:

$$\min_{f \in \mathcal{H}_k} C(f) := \frac{1}{N} \sum_{n \in [N]} [f(\mathbf{x}_n) - y_n]^2 + \sum_{j \in [d]} \|\partial_j f\|,$$
$$\|g\| = \sqrt{\frac{1}{N} \sum_{n \in [N]} |g(x_n)|^2}.$$

- ③ Infinite-dimensional exponential family (score matching):

sufficient statistics

$$p_{\theta}(\mathbf{x}) \propto e^{\langle \theta, \overbrace{\mathbf{T}(\mathbf{x})}^{\text{sufficient statistics}} \rangle} \Rightarrow p_f(\mathbf{x}) \propto e^{\langle f, k(\cdot, \mathbf{x}) \rangle_{\mathcal{H}_k}} = e^{f(\mathbf{x})} \quad (f \in \mathcal{H}_k).$$

# Solution

- Representer theorem [Zhou, 2008]:

$$f(\cdot) = \sum_{\substack{n \in [N] \\ p \in D_n}} \underbrace{a_{n,p}}_{\in \mathbb{R}} \partial^{p,0} k(\cdot, \mathbf{x}_n) \Rightarrow$$

$$\min_{\mathbf{a}} C \left( \left\{ \sum_{\substack{m \in [N] \\ q \in D_m}} a_{m,q} \partial^{p,q} k(\mathbf{x}_n, \mathbf{x}_m) \right\}_{\substack{n \in [N] \\ p \in D_n}} , \sum_{\substack{n,m \in [N] \\ p \in D_n \\ q \in D_m}} a_{n,p} a_{m,q} \partial^{p,q} k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

# Solution

- Representer theorem [Zhou, 2008]:

$$\textcolor{red}{f}(\cdot) = \sum_{\substack{n \in [N] \\ \mathbf{p} \in D_n}} \underbrace{a_{n,\mathbf{p}}}_{\in \mathbb{R}} \partial^{\mathbf{p}, \mathbf{0}} k(\cdot, \mathbf{x}_n) \Rightarrow$$

$$\min_{\mathbf{a}} C \left( \left\{ \sum_{\substack{m \in [N] \\ \mathbf{q} \in D_m}} a_{m,\mathbf{q}} \partial^{\mathbf{p}, \mathbf{q}} k(\mathbf{x}_n, \mathbf{x}_m) \right\}_{\substack{n \in [N] \\ \mathbf{p} \in D_n}} , \sum_{\substack{n,m \in [N] \\ \mathbf{p} \in D_n \\ \mathbf{q} \in D_m}} a_{n,\mathbf{p}} a_{m,\mathbf{q}} \partial^{\mathbf{p}, \mathbf{q}} k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

- RFF [Rahimi and Recht, 2007] with  $k(\mathbf{x}, \mathbf{x}') \approx \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle_{\mathbb{R}^M}$

$$f(\mathbf{x}) = \langle \textcolor{blue}{f}, k(\cdot, \mathbf{x}) \rangle_{\mathcal{H}_k} \rightarrow \hat{f}_{\mathbf{w}}(\mathbf{x}) = \langle \textcolor{blue}{w}, \phi(\mathbf{x}) \rangle_{\mathbb{R}^M},$$

Estimate  $\mathbf{w}$  by leveraging fast linear primal solvers.

# Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} e^{i\omega^T(\mathbf{x}-\mathbf{y})} d\Lambda(\omega)$$

# Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{e^{i\omega^T(\mathbf{x}-\mathbf{y})}}_{\cos(\omega^T(\mathbf{x}-\mathbf{y})) + i \sin(\omega^T(\mathbf{x}-\mathbf{y}))} d\Lambda(\omega)$$

# Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \cos(\omega^T(\mathbf{x} - \mathbf{y})) d\Lambda(\omega).$$

## Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{\cos(\omega^T(\mathbf{x} - \mathbf{y}))}_{\cos(\omega^T \mathbf{x}) \cos(\omega^T \mathbf{y}) + \sin(\omega^T \mathbf{x}) \sin(\omega^T \mathbf{y})} d\Lambda(\omega).$$

## Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{\cos(\omega^T(\mathbf{x} - \mathbf{y}))}_{\cos(\omega^T \mathbf{x}) \cos(\omega^T \mathbf{y}) + \sin(\omega^T \mathbf{x}) \sin(\omega^T \mathbf{y})} d\Lambda(\omega).$$

Trick:  $(\omega_m)_{m=1}^M \stackrel{\text{i.i.d.}}{\sim} \Lambda$ ,

$$\hat{k}(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \cos(\omega^T(\mathbf{x} - \mathbf{y})) d\Lambda_M(\omega)$$

# Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{\cos(\omega^T(\mathbf{x} - \mathbf{y}))}_{\cos(\omega^T \mathbf{x}) \cos(\omega^T \mathbf{y}) + \sin(\omega^T \mathbf{x}) \sin(\omega^T \mathbf{y})} d\Lambda(\omega).$$

Trick:  $(\omega_m)_{m=1}^M \stackrel{\text{i.i.d.}}{\sim} \Lambda$ ,

$$\begin{aligned}\hat{k}(\mathbf{x}, \mathbf{y}) &= \int_{\mathbb{R}^d} \cos(\omega^T(\mathbf{x} - \mathbf{y})) d\Lambda_M(\omega) \\ &= \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle,\end{aligned}$$

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{M}} \left[ \left( \cos(\omega_m^T \mathbf{x}) \right)_{m=1}^M, \left( \sin(\omega_m^T \mathbf{x}) \right)_{m=1}^M \right] \in \mathbb{R}^{2M}.$$

# Spectral measure & RFF features

For continuous, bounded, shift-invariant  $k$ : Bochner theorem  $\Rightarrow$

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{\cos(\omega^T(\mathbf{x} - \mathbf{y}))}_{\cos(\omega^T \mathbf{x}) \cos(\omega^T \mathbf{y}) + \sin(\omega^T \mathbf{x}) \sin(\omega^T \mathbf{y})} d\Lambda(\omega).$$

Trick:  $(\omega_m)_{m=1}^M \stackrel{\text{i.i.d.}}{\sim} \Lambda$ ,

$$\begin{aligned}\hat{k}(\mathbf{x}, \mathbf{y}) &= \int_{\mathbb{R}^d} \cos(\omega^T(\mathbf{x} - \mathbf{y})) d\Lambda_M(\omega) \\ &= \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle,\end{aligned}$$

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{M}} \left[ \left( \cos(\omega_m^T \mathbf{x}) \right)_{m=1}^M, \left( \sin(\omega_m^T \mathbf{x}) \right)_{m=1}^M \right] \in \mathbb{R}^{2M}.$$

$\widehat{\partial^{\mathbf{p}, \mathbf{q}} k}$  similarly.

# RFF applications

10-year test-of-time award (NIPS-2017).

10-year test-of-time award (NIPS-2017).

**Examples**: differential privacy preserving [Chaudhuri et al., 2011], fast function-to-function regression [Oliva et al., 2015], learning message operators in expectation propagation [Jitkrittum et al., 2015], causal discovery [Lopez-Paz et al., 2015, Strobl et al., 2019], independence testing [Zhang et al., 2017], prediction and filtering in dynamical systems [Downey et al., 2017], bandit optimization [Li et al., 2018], estimation of Gaussian mixture models [Keriven et al., 2018].

# RFF guarantee: $k$

- Kernel values

[Rahimi and Recht, 2007, Sutherland and Schneider, 2015]

$$\|k - \hat{k}\|_{L^\infty(S_M)} = \mathcal{O}_P\left(|S_M| \sqrt{\frac{\log M}{M}}\right)$$

- Kernel values

[Rahimi and Recht, 2007, Sutherland and Schneider, 2015],  
[Csörgő and Totik, 1983]

$$\|k - \hat{k}\|_{L^\infty(S_M)} = \mathcal{O}_P\left(|S_M| \sqrt{\frac{\log M}{M}}\right), |S_M| = e^{o(M)} \text{ is expected} \Rightarrow$$

# RFF guarantee: $k$

- Kernel values

[Rahimi and Recht, 2007, Sutherland and Schneider, 2015],  
[Csörgő and Totik, 1983], [Sriperumbudur and Szabó, 2015]:

$$\|k - \hat{k}\|_{L^\infty(S_M)} = \mathcal{O}_P\left(|S_M| \sqrt{\frac{\log M}{M}}\right), |S_M| = e^{o(M)} \text{ is expected} \Rightarrow$$

$$\|k - \hat{k}\|_{L^\infty(S_M)} = \mathcal{O}_{a.s.}\left(\sqrt{\frac{\log |S_M|}{M}}\right).$$

- Downstream tasks :

- ➊ Kernel ridge regression [Rudi and Rosasco, 2017], [Li et al., 2019]:
  - $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$  generalization with  $M = o(N) = \mathcal{O}\left(\sqrt{N} \log N\right)$  or less RFFs.

- Downstream tasks :

- ➊ Kernel ridge regression [Rudi and Rosasco, 2017], [Li et al., 2019]:
  - $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$  generalization with  $M = o(N) = \mathcal{O}\left(\sqrt{N} \log N\right)$  or less RFFs.
- ➋ Kernel PCA [Sriperumbudur and Sterge, 2018, Ullah et al., 2018], classification with 0-1 loss [Gilbert et al., 2018]:  $M = o(N)$  RFFs, spectrum decay.

- Kernel values ( $\mathbf{p} = \mathbf{q} = \mathbf{0}$ ):

$$\left\| \hat{k} - k \right\|_{L^\infty(S)} = \sup_{f \in \mathcal{F}} |(\Lambda_M - \Lambda)(f)|, \quad \mathcal{F} = \{ \mathfrak{f}_z : z \in S_\Delta := S - S \},$$

$$\mathfrak{f}_z(\omega) = \cos(\omega^\top z).$$

$\mathcal{F}$  is uniformly bounded:  $\sup_{z \in S_\Delta} \|\mathfrak{f}_z\|_{L^\infty(\mathbb{R}^d)} < \infty$ .

# Challenge

- Kernel values ( $\mathbf{p} = \mathbf{q} = \mathbf{0}$ ):

$$\left\| \hat{k} - k \right\|_{L^\infty(S)} = \sup_{f \in \mathcal{F}} |(\Lambda_M - \Lambda)(f)|, \quad \mathcal{F} = \{ \textcolor{red}{f_z} : z \in S_\Delta := S - S \},$$

$$\textcolor{red}{f_z}(\omega) = \cos(\omega^\top z).$$

$\mathcal{F}$  is uniformly bounded:  $\sup_{z \in S_\Delta} \|\textcolor{red}{f_z}\|_{L^\infty(\mathbb{R}^d)} < \infty$ .

- Kernel derivatives ( $[\mathbf{p}, \mathbf{q}] \neq \mathbf{0}$ ):  $\left\| \widehat{\partial^{\mathbf{p}, \mathbf{q}} k} - \partial^{\mathbf{p}, \mathbf{q}} k \right\|_{L^\infty(S)}$  with

$$\textcolor{red}{f_z}(\omega) = \omega^{\mathbf{p}} (-\omega)^{\mathbf{q}} \cos^{(|\mathbf{p} + \mathbf{q}|)} (\omega^\top z), \quad \omega^{\mathbf{p}} = \prod_{i=1}^d \omega_i^{p_i}.$$

# Challenge

- Kernel values ( $\mathbf{p} = \mathbf{q} = \mathbf{0}$ ):

$$\left\| \hat{k} - k \right\|_{L^\infty(S)} = \sup_{f \in \mathcal{F}} |(\Lambda_M - \Lambda)(f)|, \quad \mathcal{F} = \{ \textcolor{red}{f_z} : z \in S_\Delta := S - S \},$$

$$\textcolor{red}{f_z}(\omega) = \cos(\omega^\top z).$$

$\mathcal{F}$  is uniformly bounded:  $\sup_{z \in S_\Delta} \|f_z\|_{L^\infty(\mathbb{R}^d)} < \infty$ .

- Kernel derivatives ( $[\mathbf{p}, \mathbf{q}] \neq \mathbf{0}$ ):  $\left\| \widehat{\partial^{\mathbf{p}, \mathbf{q}} k} - \partial^{\mathbf{p}, \mathbf{q}} k \right\|_{L^\infty(S)}$  with

$$\textcolor{red}{f_z}(\omega) = \omega^{\mathbf{p}} (-\omega)^{\mathbf{q}} \cos^{(|\mathbf{p} + \mathbf{q}|)} (\omega^\top z), \quad \omega^{\mathbf{p}} = \prod_{i=1}^d \omega_i^{p_i}.$$

$\mathcal{F}$  is of polynomial growth.

Kernel derivatives [Szabó and Sriperumbudur, 2019]:

- Same fast rate as for kernel values (unbounded emp. processes).

## RFF guarantee: $\partial^{p,q} k$

Kernel derivatives [Szabó and Sriperumbudur, 2019]:

- Same fast rate as for kernel values (unbounded emp. processes).
- Bernstein condition on  $\Lambda$ :  $d = 1$ ,  $f_\Lambda(\omega) \propto e^{-\omega^{2\ell}} \Rightarrow p + q \leq 2\ell : \checkmark$

RFF guarantee:  $\partial^{\mathbf{p}, \mathbf{q}} k$

Now:  $\alpha$ -exponential Orlicz spectrum (Bernstein  $\Rightarrow$  sub-exponential)

$f_\Lambda$  spectrum with at least  $e^{-\|\omega\|_2^\alpha}$  tail decay,  $\alpha > 0$ .

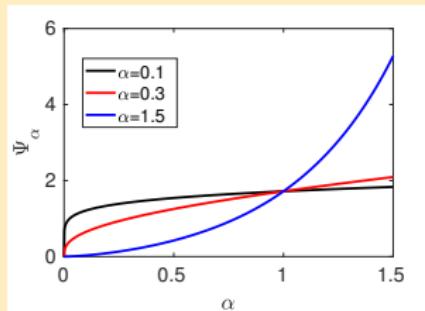
- Examples: sub-Gaussian ( $\alpha = 2$ ), sub-exponential ( $\alpha = 1$ ).

# RFF guarantee: $\partial^{\mathbf{p}, \mathbf{q}} k$

Now:  $\alpha$ -exponential Orlicz spectrum (Bernstein  $\Rightarrow$  sub-exponential)

$f_\Lambda$  spectrum with at least  $e^{-\|\omega\|_2^\alpha}$  tail decay,  $\alpha > 0$ .

- Examples: sub-Gaussian ( $\alpha = 2$ ), sub-exponential ( $\alpha = 1$ ).
- $L_{\Psi_\alpha} := \left\{ \Lambda : \|\Lambda\|_{\Psi_\alpha} := \inf \left\{ c > 0 : \mathbb{E}_{\omega \sim \Lambda} \Psi_\alpha \left( \frac{\|\omega\|_2}{c} \right) \leq 1 \right\} < +\infty \right\}$ .
- $\Psi_\alpha : x \in \mathbb{R}^{\geq 0} \mapsto e^{x^\alpha} - 1 \in \mathbb{R}^{\geq 0}$ .



# Main result

Blanket assumptions:

- $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  continuous, bounded, shift-invariant kernel with  $\alpha$ -exponential Orlicz spectrum ( $\alpha > 0$ ),
- $\mathbf{p}, \mathbf{q} \in \mathbb{N}^d$ .

# Main result

Blanket assumptions:

- $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  continuous, bounded, shift-invariant kernel with  $\alpha$ -exponential Orlicz spectrum ( $\alpha > 0$ ),
- $\mathbf{p}, \mathbf{q} \in \mathbb{N}^d$ .

Finite sample guarantee [Chamakh et al., 2019],  $\Rightarrow$

Fast rates

$$\left\| \partial^{\mathbf{p}, \mathbf{q}} k - \widehat{\partial^{\mathbf{p}, \mathbf{q}} k} \right\|_{L^\infty(S_M)} = \mathcal{O}_{a.s.} \left( \sqrt{\frac{\log |S_M|}{M}} \right), \Rightarrow |S_M| = e^{o(M)} \sqrt{M}$$

For tensor product kernels:

If

- $k_i \leftrightarrow \Lambda_i \in L_{\Psi_{\alpha_i}}$

For tensor product kernels:

If

- $k_i \leftrightarrow \Lambda_i \in L_{\Psi_{\alpha_i}}$
- $k(\mathbf{x}, \mathbf{y}) = \prod_{i \in [d]} k_i(x_i, y_i)$ , i.e.  $\Lambda = \otimes_{i \in [d]} \Lambda_i$ ,

For tensor product kernels:

If

- $k_i \leftrightarrow \Lambda_i \in L_{\Psi_{\alpha_i}}$  and
- $k(\mathbf{x}, \mathbf{y}) = \prod_{i \in [d]} k_i(x_i, y_i)$ , i.e.  $\Lambda = \otimes_{i \in [d]} \Lambda_i$ ,

then  $\Lambda \in L_{\Psi_\alpha}$  with  $\alpha = \min_{i \in [d]} \alpha_i$ .

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma(\frac{1}{\alpha})} e^{-\frac{ \omega ^\alpha}{\beta}}$	$\alpha$

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx.$$

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma(\frac{1}{\alpha})} e^{-\frac{ \omega ^\alpha}{\beta}}$	$\alpha$
variance Gamma	$\frac{\sigma^{2b} \omega ^{b-\frac{1}{2}} K_{b-\frac{1}{2}}(\sigma \omega )}{\sqrt{\pi}\Gamma(b)(2\sigma)^{b-\frac{1}{2}}}$	1

$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx$ .  $K_b$ : modified Bessel function of 2nd kind and order  $b$ .

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma(\frac{1}{\alpha})} e^{-\frac{ \omega ^\alpha}{\beta}}$	$\alpha$
variance Gamma	$\frac{\sigma^{2b} \omega ^{b-\frac{1}{2}} K_{b-\frac{1}{2}}(\sigma \omega )}{\sqrt{\pi}\Gamma(b)(2\sigma)^{b-\frac{1}{2}}}$	1
hyperbolic secant	$\frac{1}{2} \operatorname{sech}\left(\frac{\pi}{2}\omega\right)$	1

$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx$ .  $K_b$ : modified Bessel function of 2nd kind and order  $b$ .  $\operatorname{sech}(x) = \frac{1}{\cosh(x)} = \frac{2}{e^x + e^{-x}}$ .

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma(\frac{1}{\alpha})} e^{-\frac{ \omega ^\alpha}{\beta}}$	$\alpha$
variance Gamma	$\frac{\sigma^{2b} \omega ^{b-\frac{1}{2}} K_{b-\frac{1}{2}}(\sigma \omega )}{\sqrt{\pi}\Gamma(b)(2\sigma)^{b-\frac{1}{2}}}$	1
hyperbolic secant	$\frac{1}{2} \operatorname{sech}\left(\frac{\pi}{2}\omega\right)$	1
logistic	$\frac{e^{-\frac{\omega}{s}}}{s[1+e^{-\frac{\omega}{s}}]^2} = \frac{1}{4s} \operatorname{sech}^2\left(\frac{\omega}{2s}\right)$	1

$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx$ .  $K_b$ : modified Bessel function of 2nd kind and order  $b$ .  $\operatorname{sech}(x) = \frac{1}{\cosh(x)} = \frac{2}{e^x + e^{-x}}$ . 23 examples in TR.

# Kernel examples $\leftrightarrow$ spectrum ( $b > \frac{1}{2}$ , $s > 0$ )

Kernel	$k(x, y)$	Spectrum
Gaussian	$e^{-\frac{\sigma^2(x-y)^2}{2}}$	Gaussian
Cauchy / inverse quadric	$\frac{\sigma^2}{\sigma^2 + (x-y)^2}$	Laplace
inverse multiquadric	$\left[ \frac{\sigma^2}{\sigma^2 + (x-y)^2} \right]^b$	variance Gamma
-	$\text{sech}(x - y)$	hyperbolic secant
-	$\frac{\pi s(x-y)}{\sinh(\pi s(x-y))}$	logistic

## Summary

- Focus: RFF-based acceleration for derivatives.
- Result:  $\alpha$ -exponential Orlicz spectrum  $\Rightarrow$  fast rates ( $\forall \mathbf{p}, \mathbf{q}$  order),
- Preprint on HAL: **Orlicz Random Fourier Features**.
- Future: downstream tasks.

# Summary

- Focus: RFF-based acceleration for derivatives.
- Result:  $\alpha$ -exponential Orlicz spectrum  $\Rightarrow$  fast rates ( $\forall \mathbf{p}, \mathbf{q}$  order),
- Preprint on HAL: **Orlicz Random Fourier Features**.
- Future: downstream tasks.



**Acknowledgments:** This research benefited from the support of the [Chair Stress Test](#), RISK Management and Financial Steering, led by the French Ecole polytechnique and its Foundation and sponsored by BNP Paribas.

# Summary

- Focus: RFF-based acceleration for derivatives.
- Result:  $\alpha$ -exponential Orlicz spectrum  $\Rightarrow$  fast rates ( $\forall \mathbf{p}, \mathbf{q}$  order),
- Preprint on HAL: **Orlicz Random Fourier Features**.
- Future: downstream tasks.



RISK Management and Financial Steering

**Acknowledgments:** This research benefited from the support of the [Chair Stress Test](#), RISK Management and Financial Steering, led by the French Ecole polytechnique and its Foundation and sponsored by BNP Paribas.

# Contents

- Kernel examples with  $\alpha$ -exponential Orlicz spectrum.
- Proof idea.

# Kernel examples with $\alpha$ -exp. Orlicz spectrum: $d = 1$

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2} e^{-\sigma \omega }$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma(\frac{1}{\alpha})} e^{-\frac{ \omega ^\alpha}{\beta}}$	$\alpha$
variance Gamma	$\frac{\sigma^{2b} \omega ^{b-\frac{1}{2}} K_{b-\frac{1}{2}}(\sigma \omega )}{\sqrt{\pi}\Gamma(b)(2\sigma)^{b-\frac{1}{2}}}$	1
Weibull (S)	$\frac{s}{2\lambda} \left(\frac{ \omega }{\lambda}\right)^{s-1} e^{-\left(\frac{ \omega }{\lambda}\right)^s}$	$s$
exponentiated exponential (S)	$\frac{\alpha}{2\lambda} \left(1 - e^{-\frac{ \omega }{\lambda}}\right)^{\alpha-1} e^{-\frac{ \omega }{\lambda}}$	1

$I_a(z) = \sum_{n \in \mathbb{N}} \frac{1}{n! \Gamma(n+a+1)} \left(\frac{z}{2}\right)^{2n+a}$ ,  $K_a(z) = \frac{\pi}{2} \frac{I_{-a}(z) - I_a(z)}{\sin(a\pi)}$  for  $z \in \mathbb{R}$  and non-integer  $a$ ; when  $a$  is an integer the limit is taken.

# Kernel examples with $\alpha$ -exponential Orlicz spectrum - 2

Spectrum	$f_\Lambda(\omega)$	$\alpha$
exponentiated Weibull (S)	$\frac{\alpha s}{2\lambda} \left( \frac{ \omega }{\lambda} \right)^{s-1} \left[ 1 - e^{-\left( \frac{ \omega }{\lambda} \right)^s} \right]^{\alpha-1} \times s \\ \times e^{-\left( \frac{ \omega }{\lambda} \right)^s}$	$s$
Nakagami (S)	$\frac{m^m}{\Gamma(m)\Omega^m}  \omega ^{2m-1} e^{-\frac{m\omega^2}{\Omega}}$	2
chi-squared (S)	$\frac{1}{2^{\frac{s}{2}+1}\Gamma(\frac{s}{2})}  \omega ^{\frac{s}{2}-1} e^{-\frac{ \omega }{2}}$	1
Erlang (S)	$\frac{\lambda^s  \omega ^{s-1} e^{-\lambda  \omega }}{2(s-1)!}$	1
Gamma (S)	$\frac{1}{2\Gamma(s)\theta^s}  \omega ^{s-1} e^{-\frac{ \omega }{\theta}}$	1
generalized Gamma (S)	$\frac{p/a^D}{2\Gamma(\frac{D}{p})}  \omega ^{D-1} e^{-\left( \frac{ \omega }{a} \right)^p}$	$p$

# Kernel examples with $\alpha$ -exponential Orlicz spectrum - 3

Spectrum	$f_\Lambda(\omega)$	$\alpha$
Rayleigh (S)	$\frac{ \omega }{2\sigma^2} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Maxwell-Boltzmann (S)	$\frac{1}{\sqrt{2\pi}} \frac{\omega^2 e^{-\frac{\omega^2}{2a^2}}}{a^3}$	2
chi (S)	$\frac{1}{2^{\frac{s}{2}} \Gamma(\frac{s}{2})}  \omega ^{s-1} e^{-\frac{\omega^2}{2}}$	2
exponential-logarithmic (S)	$-\frac{1}{2 \log(p)} \frac{\beta(1-p)e^{-\beta \omega }}{1-(1-p)e^{-\beta \omega }}$	1
Weibull-logarithmic (S)	$-\frac{1}{2 \log(p)} \frac{\alpha\beta(1-p) \omega ^{\alpha-1}e^{-\beta \omega ^\alpha}}{1-(1-p)e^{-\beta \omega ^\alpha}}$	$\alpha$
Gamma/Gompertz (S)	$\frac{bse^{b \omega }\beta^s}{2(\beta-1+e^{b \omega })^{s+1}}$	$bs$

# Kernel examples with $\alpha$ -exponential Orlicz spectrum - 4

Spectrum	$f_\Lambda(\omega)$	$\alpha$
hyperbolic secant	$\frac{1}{2} \operatorname{sech}\left(\frac{\pi}{2}\omega\right)$	1
logistic	$\frac{e^{-\frac{\omega}{s}}}{s\left[1+e^{-\frac{\omega}{s}}\right]^2} = \frac{1}{4s} \operatorname{sech}^2\left(\frac{\omega}{2s}\right)$	1
normal-inverse Gaussian	$\frac{\alpha\delta K_1(\alpha\sqrt{\delta^2+\omega^2})}{\pi\sqrt{\delta^2+\omega^2}} e^{\delta\alpha}$	1
hyperbolic	$\frac{1}{2\delta K_1(\delta\alpha)} e^{-\alpha\sqrt{\delta^2+\omega^2}}$	1
generalized hyperbolic	$\frac{(\alpha/\delta)^\lambda}{\sqrt{2\pi}K_\lambda(\delta\gamma)} \frac{K_{\lambda-\frac{1}{2}}(\alpha\sqrt{\delta^2+\omega^2})}{\left(\frac{\sqrt{\delta^2+\omega^2}}{\alpha}\right)^{\frac{1}{2}-\lambda}}$	1

$$\operatorname{sech}(x) = \frac{1}{\cosh(x)} = \frac{2}{e^x + e^{-x}}.$$

Decomposition into 3 terms:

- ① Unbounded part: Talagrand & Hoffman-Jorgensen inequalities.
- ② Bounded part: Klein-Rio inequality & Dudley entropy integral bound.
- ③ Truncation: bound on the incomplete Gamma function.

-  Chamakh, L., Gobet, E., and Szabó, Z. (2019).  
Orlicz random Fourier features.  
Technical report.  
(<https://hal.archives-ouvertes.fr/hal-02418576>).
-  Chaudhuri, K., Monteleoni, C., and Sarwate, A. D. (2011).  
Differentially private empirical risk minimization.  
*Journal of Machine Learning Research*, 12:1069–1109.
-  Csörgö, S. and Totik, V. (1983).  
On how long interval is the empirical characteristic function uniformly consistent?  
*Acta Scientiarum Mathematicarum*, 45:141–149.
-  Downey, C., Hefny, A., Boots, B., Li, B., and Gordon, G. (2017).  
Predictive state recurrent neural networks.  
In *Advances in Neural Information Processing Systems (NIPS)*, pages 6053–6064.

-  Duijkers, R., Tóth, R., Piga, D., and Laurain, V. (2014). Shrinking complexity of scheduling dependencies in LS-SVM based LPV system identification.  
In *IEEE Conference on Decision and Control*, pages 2561–2566.
-  Gilbert, A., Tewari, A., and Sung, Y. (2018). But how does it work in theory? Linear SVM with random features.  
In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 3379–3388.
-  Jitkrittum, W., Gretton, A., Heess, N., Eslami, A., Lakshminarayanan, B., Sejdinovic, D., and Szabó, Z. (2015). Kernel-based just-in-time learning for passing expectation propagation messages.  
In *Conference on Uncertainty in Artificial Intelligence (UAI)*, pages 405–414.
-  Keriven, N., Bourrier, A., Gribonval, R., and Pérez, P. (2018).

Sketching for large-scale learning of mixture models.

*Information and Inference: A Journal of the IMA*, 7:447–508.

-  Lauer, F., Le, V. L., and Bloch, G. (2012).  
Learning smooth models of nonsmooth functions via convex optimization.  
In *International Workshop on Machine Learning for Signal Processing (IEEE-MLSP)*.
-  Li, L., Jamieson, K., DeSalvo, G., Rostamizadeh, A., and Talwalkar, A. (2018).  
Hyperband: A novel bandit-based approach to hyperparameter optimization.  
*Journal of Machine Learning Research*, 18(185):1–52.
-  Li, Z., Ton, J.-F., Ogle, D., and Sejdinovic, D. (2019).  
A unified analysis of random Fourier features.  
In *International Conference on Machine Learning (ICML; PMLR)*.

-  Lopez-Paz, D., Muandet, K., Schölkopf, B., and Tolstikhin, I. (2015).  
Towards a learning theory of cause-effect inference.  
*International Conference on Machine Learning (ICML)*, 37:1452–1461.
-  Oliva, J., Neiswanger, W., Póczos, B., Xing, E., and Schneider, J. (2015).  
Fast function to function regression.  
In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, pages 717–725.
-  Rahimi, A. and Recht, B. (2007).  
Random features for large-scale kernel machines.  
In *Advances in Neural Information Processing Systems (NIPS)*, pages 1177–1184.
-  Rosasco, L., Santoro, M., Mosci, S., Verri, A., and Villa, S. (2010).  
A regularization approach to nonlinear variable selection.

In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 9, pages 653–660.

-  Rosasco, L., Villa, S., Mosci, S., Santoro, M., and Verri, A. (2013).  
Nonparametric sparsity and regularization.  
*Journal of Machine Learning Research*, 14:1665–1714.
-  Rudi, A. and Rosasco, L. (2017).  
Generalization properties of learning with random features.  
In *Advances in Neural Information Processing Systems (NIPS)*, pages 3218–3228.
-  Sriperumbudur, B. and Sterge, N. (2018).  
Approximate kernel PCA using random features:  
Computational vs. statistical trade-off.  
Technical report, Pennsylvania State University.  
(<https://arxiv.org/abs/1706.06296>).
-  Sriperumbudur, B. K., Fukumizu, K., Gretton, A., Hyvärinen, A., and Kumar, R. (2017).

Density estimation in infinite dimensional exponential families.  
*Journal of Machine Learning Research*, 18(57):1–59.

-  Sriperumbudur, B. K. and Szabó, Z. (2015).  
Optimal rates for random Fourier features.  
In *Advances in Neural Information Processing Systems (NIPS)*,  
pages 1144–1152.
-  Strathmann, H., Sejdinovic, D., Livingstone, S., Szabó, Z.,  
and Gretton, A. (2015).  
Gradient-free Hamiltonian Monte Carlo with efficient kernel  
exponential families.  
In *Advances in Neural Information Processing Systems (NIPS)*,  
pages 955–963.
-  Strobl, E. V., Zhang, K., and Visweswaran, S. (2019).  
Approximate kernel-based conditional independence tests for  
fast non-parametric causal discovery.  
*Journal of Causal Inference*, 7(1).  
(<https://doi.org/10.1515/jci-2018-0017>).

-  Sutherland, D. J. and Schneider, J. (2015).  
On the error of random Fourier features.  
In *Conference on Uncertainty in Artificial Intelligence (UAI)*, pages 862–871.
-  Szabó, Z. and Sriperumbudur, B. K. (2019).  
On kernel derivative approximation with random Fourier features.  
In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 89, pages 827–836.
-  Ullah, E., Mianjy, P., Marinov, T. V., and Arora, R. (2018).  
Streaming kernel PCA with  $\tilde{O}(\sqrt{n})$  random features.  
In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 7311–7321.
-  Ying, Y., Wu, Q., and Campbell, C. (2012).  
Learning the coordinate gradients.  
*Advances in Computational Mathematics*, 37:355–378.

-  Zhang, Q., Filippi, S., Gretton, A., and Sejdinovic, D. (2017). Large-scale kernel methods for independence testing. *Statistics and Computing*, pages 1–18.
-  Zhou, D.-X. (2008). Derivative reproducing properties for kernel methods in learning theory. *Journal of Computational and Applied Mathematics*, 220:456–463.